Matter Wave Scattering from Ultracold Atoms in an Optical Lattice

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We study matter wave scattering from an ultracold, many body atomic system trapped in an optical lattice. We determine the angular cross section that a matter wave probe sees and show that it is strongly affected by the many body phase, superfluid or Mott insulator, of the target lattice. We determine these cross sections analytically in the first Born approximation, and we examine the variation at intermediate points in the phase transition by numerically diagonalizing the Bose Hubbard Hamiltonian for a small lattice. We show that matter wave scattering offers a convenient method for non-destructively probing the quantum many body phase transition of atoms in an optical lattice.

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Ultracold atoms in an optical lattice form an optical crystal that permits the clean implementation of fundamental models of condensed matter physics to a degree unheard of in other systems. The physical parameters that characterize this system, namely the depth of the lattice and the interactions of the atoms in the lattice, are experimentally tunable so that it is possible to probe the atoms' behavior controllably from non-interacting single particle mechanics to strongly interacting, many body physics [1, 2, 3]. Of particular interest are the many body theories of quantum phase transitions, whose predictions can be observed in such a system.

The superfluid to Mott insulator phase transition has been probed experimentally by studying the interference of clouds of atoms expanding freely out of an optical lattice [4]. This method provides information about the correlation properties of the ground state of the cold atom system, but does not depend on the excitation spectrum of the lattice, which is essential to study the superfluid fraction [5]. Bragg spectroscopy has been combined with this method in order to examine the excitation spectrum [6]; nevertheless, it requires the destruction of the sample under examination. More recently, it has been proposed theoretically that the on-site number statistics can be probed by observing light scattered into an optical cavity [7]. Very recently, light scattering from optical lattice systems has been analyzed to determine the effect of the many body phase on the scattering cross section of a photon due to interactions with a lattice [8]. Very little attention has been paid to the interaction of matter waves with these optical crystals. Theoretical work has been done emphasizing the impact of disordered atoms in a periodic potential on scattering of photons and particles [9]. We are interested, however, in the impact of the many body phase on matter wave scattering.

The scattering of matter waves from a lattice system provides a very useful technique to probe the many body phase transition both because it does not require the destruction of the lattice under examination and because it depends strongly on the excitation spectrum of the target. This is critical to probe superfluidity and the dynamics of the lattice, beyond analysis of ground state properties. In addition, the simple form of the interaction between a slow-moving probe atom and the atoms in the lattice emphasizes structure that depends on the many body properties of the lattice. As we will show, the differential cross section is a highly suitable quantity for the distinction between the Mott insulating and superfluid phases.

Our objective has been to study the scattering patterns of matter waves due to passage through ultracold atoms trapped in a uniform optical lattice. The scattering target is well modeled by the Bose Hubbard Hamiltonian, H_{BH} [1],

$$\hat{H}_{\mathrm{BH}} = -J \sum_{\langle \boldsymbol{R},\boldsymbol{R'}\rangle} \hat{a}^{\dagger}_{\boldsymbol{R}} \hat{a}_{\boldsymbol{R'}} + \frac{1}{2} U \sum_{\boldsymbol{R}} \hat{n}_{\boldsymbol{R}} (\hat{n}_{\boldsymbol{R}} - 1) \qquad (1)$$

The probe is a free particle of mass, m, with Hamiltonian, $H_P = \hat{p}^2/2m$, which does not interact with the confining light of the lattice. We require low-energy probes that avoid interband excitations of atoms in the lattice. In this case, s-wave scattering is dominant, and we may treat the interaction between the probe and each lattice atom as a pseudopotential with scattering length, a_s. The total interaction potential is $\hat{V} = \sum_j \frac{2\pi\hbar^2}{m} a_s \delta(\hat{\boldsymbol{r}} - \hat{\boldsymbol{r}}_j)$ [10]. The operators $\hat{\boldsymbol{r}}$ and $\hat{\boldsymbol{r}}_j$ give the positions of the probe and the j^{th} lattice atom, respectively. The full Hamiltonian for the scattering interaction is $\hat{H} = \hat{H}_{\mathrm{P}} + \hat{H}_{\mathrm{BH}} + \hat{V}$.

The states of the lattice before and after scattering of a probe atom are many body states of the N atoms in the lattice. The particular ground state in the lattice depends on the relative sizes of the the interaction strength, U, and the tunneling matrix element, J, appearing in the Bose Hubbard model. For weak repulsion between the atoms in the lattice, the atoms will delocalize and the superfluid fraction will increase to one as the interaction strength goes to zero [5]. As the repulsion between the atoms in the lattice becomes large compared to the tunneling matrix element, the atoms will localize, the

superfluid fraction will go to zero, and a gap will open in the excitation spectrum, giving rise to the Mott insulator state. It is possible to alter the interaction strength between the atoms in the lattice by adjusting the depth of the lattice, or by manipulating the scattering length of lattice atom collisions through a Feshbach resonance. It is best for the purpose of probing the many body phase of the lattice to retain a constant lattice depth so that the scattering patterns are not trivially affected by the changing density profile associated with a changing lattice potential.

The incident probe wavefunction is in the plane wave state, $|\boldsymbol{k}_0\rangle$, with energy, $\hbar^2 k_0^2/(2m)$. The target is initially in the ground state, $|n_0\rangle$, of the Bose Hubbard Hamiltonian, with energy, E_{n_0}. We consider the cross section for a transfer of momentum $\boldsymbol{\kappa} = \boldsymbol{k_0} - \boldsymbol{k}$ from the probe to the lattice. This is associated with a change of the state of the atoms in the lattice to a potentially excited state, $|n\rangle$. The energy gained by the lattice atoms is related to the energy lost by the probe by $E_n - E_{n_0} = \frac{\hbar^2}{2m}\left(k_0^2 - k^2\right)$. In the first Born approximation, the scattering cross section separates into two factors. One of which is determined by the binary interaction between the probe and each target. The other is determined solely by the structure of the target [11]. This is true for general choices of the interaction potential. In the case of the pseudopotential, the scattered wave from an individual target is a structureless spherical wave, and the total angular cross section is given by

$$\frac{d\sigma}{d\Omega} = a_s^2 \sum_n \sqrt{1 - \frac{E_n - E_{n_0}}{\hbar^2 k_o^2/(2m)}} \left| \langle n | \sum_{j=1}^{N} e^{i\boldsymbol{\kappa}\cdot\hat{\boldsymbol{r}}_j} |n_o\rangle \right|^2 . \tag{2}$$

The cross section vanishes when the quantity under the square root becomes less than zero, due to energy conservation. The momentum transfer, $\boldsymbol{\kappa}$, depends on the index, n, of the final state through the dependence on the final wavenumber, k, of the probe. A natural choice of units for the cross section is the square of the scattering length, a_s. The quantity under the square root diminishes the contribution of scattering into final target states at progressively higher energy. The matrix element of the momentum boost gives the transition amplitude between the ground and excited states of the target due to a transfer of momentum, $\boldsymbol{\kappa}$, from the probe. When the interaction strength between the lattice atoms, U, is very large or small compared to the tunneling matrix element, J, it is possible to evaluate the cross section in (2) analytically. At intermediate values of U/J, we will numerically diagonalize the Hamiltonian to evaluate the cross section.

For very weak interactions, we may treat the target as a condensate in the lowest energy Bloch wave, $\psi_0(\boldsymbol{r})$, of the lowest band of the lattice. Designating the operator that creates particles in this state by $\hat{\psi}_0^\dagger = \int d^3r\, \psi_0(\boldsymbol{r})\hat{\psi}^\dagger(\boldsymbol{r})$, the ground state of the pure superfluid target is

$$|n_o\rangle = \frac{1}{\sqrt{N!}} \left(\frac{\hat{\psi}_0^\dagger}{\sqrt{N_L}} \right)^N |0\rangle . \tag{3}$$

N is the number of atoms in the lattice, N_L is the number of lattice sites. In order to calculate the matrix element appearing in (2) for momentum transfer, $\boldsymbol{\kappa}$, to the target, it is useful to express the many body operator in terms of the density, $\hat{n}(\boldsymbol{r}) = \hat{\psi}^\dagger(\boldsymbol{r})\hat{\psi}(\boldsymbol{r})$, using $\sum_{j=1}^N e^{i\boldsymbol{\kappa}\cdot\hat{\boldsymbol{r}}_j} = \int d^3r\; e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}}\,\hat{n}(\boldsymbol{r})$.

A convenient basis for the target in the non-interacting case is a designation of the number of atoms in each mode of the lowest band of the lattice. Matrix elements of the form, $\langle n|\,\hat{n}(\boldsymbol{r})\,|n_o\rangle$, are non-zero if at most one atom in the condensate has been excited out of the lowest energy Bloch wave. We only need to consider final states of the form, $|n\rangle = \hat{\psi}_{\boldsymbol{q}}^\dagger |\xi\rangle$, where $|\xi\rangle$ represents $N-1$ atoms in the ground state and $\hat{\psi}_{\boldsymbol{q}}^\dagger$ creates particles in the $\boldsymbol{q} \neq 0$ mode. The matrix element then takes the form

$$\langle n|\,\hat{n}(\boldsymbol{r})\,|n_o\rangle = \frac{\sqrt{N}}{N_L}\psi_{\boldsymbol{q}}^*(\boldsymbol{r})\psi_0(\boldsymbol{r}) \tag{4}$$

The energy difference of the target state, when only a single atom is excited, reduces to the single particle energy difference between the two Bloch waves, $E_n - E_{n_0} = \varepsilon(\boldsymbol{q}) - \varepsilon(0)$, where $\varepsilon(\boldsymbol{q})$ is the energy of a single atom in the specified Bloch mode of the lattice, $\boldsymbol{q}$, corresponding to the excitation. The $|n\rangle = |n_o\rangle$ case must be handled separately. The result we obtain for the diagonal matrix element is

$$\langle n_o|\,\hat{n}(\boldsymbol{r})\,|n_o\rangle = \frac{N}{N_L}\left|\psi_0(\boldsymbol{r})\right|^2 . \tag{5}$$

We may now write down an expression for the cross section in (2) in the case of a superfluid ground state using the above results for the matrix element of the density operator,

$$\frac{1}{a_s^2}\frac{d\sigma}{d\Omega} = N(N-1)\left| \int d^3r\; e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}}\frac{|\psi_0(\boldsymbol{r})|^2}{N_L}\right|^2$$
$$+ N a_s^2 \sum_{\boldsymbol{q}} \sqrt{1 - \frac{\varepsilon(\boldsymbol{q}) - \varepsilon(0)}{\hbar^2 k_o^2/2m}} \left| \int d^3r\; e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}}\frac{\psi_{\boldsymbol{q}}^*(\boldsymbol{r})\psi_0(\boldsymbol{r})}{N_L}\right|^2 . \tag{6}$$

The $\boldsymbol{q} = 0$ component of the cross section gives Bragg peaks due to the coherent overlap of elastically scattered waves from each individual lattice site. The scale of the elastic scattering that gives rise to the Bragg peaks can be determined by considering scattering in the forward direction ($\boldsymbol{\kappa} = 0$). There we find that the central Bragg peak has a height $\frac{1}{a_s^2}\frac{d\sigma}{d\Omega} = N^2$.

The sum in the second term is over the modes of the lowest band of the lattice. This term is exactly N times

the single target cross section. This includes the elastic single target channel, $\boldsymbol{q} = 0$. We can estimate the scale of this term by considering the case in which the probe energy significantly exceeds the bandwidth of the lowest band, but is insufficient to excite atoms into higher bands. The energy of the probe and depth of the lattice are conveniently specified in units of the recoil energy, $E_r = \hbar^2 k_L^2/(2m_T)$, for photons with wavenumber k_L and lattice atoms of mass, m_T. This condition is readily achieved for a typical lattice depth of $V_o = 15E_r$, in which the width of the lowest band is $0.03E_r$ and the band gap between the first and second bands is $6.28E_r$. When we approximate the final wavenumber of the probe to be equal to the initial wavenumber, the second term in (6) becomes Na_s^2.

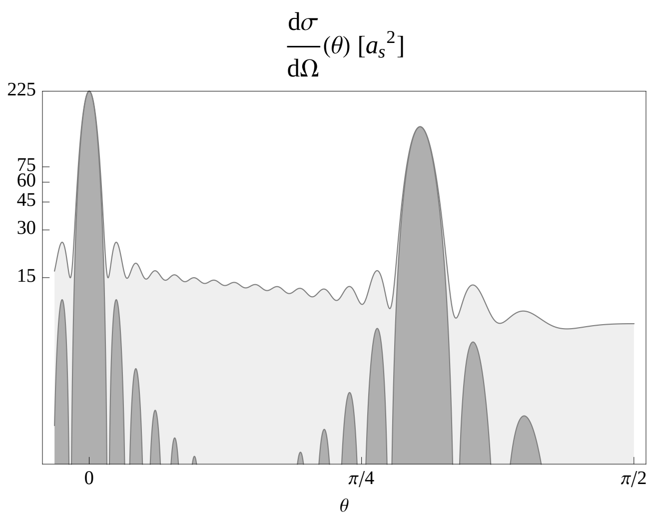

FIG. 1: The analytic results for the superfluid (light gray) and Mott insulator (dark gray) differential cross sections for a sample lattice in 1D with 15 atoms and 15 sites. These are shown on a log scale in order to draw attention to the absence of inelastic scattering from the Mott insulator. The cross section is for a probe with energy $6E_r$ and a lattice depth of $V_o/E_r = 15$.

There are two major features to the scattering from a superfluid: narrow elastic Bragg peaks that scale as N^2 and a superimposed inelastic background that scales as N. Fig. 1, which shows the differential cross sections for the superfluid (light gray) and the Mott insulator (dark gray), illustrates this behavior for a one-dimensional lattice arranged perpendicular to the incident probe wavevector. We consider the angle of deviation in the plane of the lattice. As the number of lattice sites increases, the width of the elastic peaks will become increasingly narrow. Away from the sharp Bragg peaks, the inelastic background is readily identifiable. This background emerges due to the availability of excited state modes to the condensate. The scattering behavior is qualitatively different when the interaction strength between atoms in the lattice becomes very large.

As the atoms in the lattice repel each other more strongly ($U/J \to \infty$), the superfluid fraction decreases, and the atoms become localized within individual wells of the lattice. For a sufficiently strong interaction, the Mott insulator state forms, and the ground state of the target can be represented by the number of atoms at each lattice site, $|n_o\rangle = \left|\bar{n}_{\boldsymbol{R}_1}, ..., \bar{n}_{\boldsymbol{R}_{N_L}}\right\rangle$. A uniform lattice will have $\bar{n} = N/N_L$ atoms per site for integer $\bar{n}$. We must determine the matrix element $\langle n|\, \hat{n}(\boldsymbol{r})\, |n_o\rangle$ for this ground state. This is most easily done by expanding the density operator in a Wannier basis, using the Wannier function for the lowest band of the lattice, $w(\boldsymbol{r})$. Then $\hat{n}(\boldsymbol{r}) = \sum_{\boldsymbol{R}_1,\boldsymbol{R}_2} w^*(\boldsymbol{r}-\boldsymbol{R}_1)w(\boldsymbol{r}-\boldsymbol{R}_2)\hat{a}^\dagger_{\boldsymbol{R}_1}\hat{a}_{\boldsymbol{R}_2}$. Each term in the sum gives the contribution of the process in which a single target atom is scattered from one site to another by the probe. The $\boldsymbol{R}_1 = \boldsymbol{R}_2$ term is the elastic channel in which the state of the target is unchanged, $|n\rangle = |n_o\rangle$. Inelastic scattering corresponds to $\boldsymbol{R}_1 \neq \boldsymbol{R}_2$. The matrix element of the final state of the target, in which one atom has been displaced from $\boldsymbol{R}'$ to $\boldsymbol{R}$, is given by $\langle n|\, \hat{n}(\boldsymbol{r})\, |n_o\rangle = \sqrt{(\bar{n}+1)\bar{n}}\, w^*(\boldsymbol{r}-\boldsymbol{R})w(\boldsymbol{r}-\boldsymbol{R}')$. The energy cost associated with displacing one atom from the uniform ground state is the interaction strength, U, which is also the size of the Mott insulator gap. These results permit us to write the explicit expression for the scattering cross section of the Mott insulator target,

$$\frac{1}{a_s^2}\frac{d\sigma}{d\Omega} = \bar{n}^2 \left|\sum_{\boldsymbol{R}} e^{i\boldsymbol{\kappa}\cdot\boldsymbol{R}}\right|^2 \times \left|\int d^3r\; e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}}\, |w(\boldsymbol{r})|^2\right|^2 + \bar{n}(\bar{n}+1)\sqrt{1 - \frac{U}{\hbar^2 k_o^2/2m}} \times \sum_{\boldsymbol{R}\neq\boldsymbol{R}'} \left|\int d^3r\; e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}} w^*(\boldsymbol{r}-\boldsymbol{R})w(\boldsymbol{r}-\boldsymbol{R}')\right|^2 . \quad (7)$$

The sum over lattice sites in the first term takes a maximum value when the momentum transferred from the probe is a reciprocal lattice vector, with $\boldsymbol{\kappa}\cdot\boldsymbol{R}$ an integer multiple of 2π. As the number of lattice sites increases, the elastic Bragg peaks become increasingly sharp. In addition, there is an approximately Gaussian envelope due to the Fourier transform of the Wannier function.

We can examine the $\boldsymbol{\kappa} = 0$ case of forward scattering, as we did for the superfluid cross section. We see that the central peak has a height $\frac{1}{a_s^2}\frac{d\sigma}{d\Omega} = N^2$. The elastic scattering from the Mott insulator overlaps strongly with the elastic scattering given by the superfluid; however, inelastic scattering from the Mott insulator phase is strongly suppressed (see Fig. 1). In particular, if the incident energy of the probe is less than the Mott insulator gap, the inelastic scattering vanishes completely. For probe energies exceeding the gap, the inelastic scattering is also negligible under the tight binding approximation. In that case, the integral in the inelastic part of the cross

section in (7) is negligible when $\boldsymbol{R} \neq \boldsymbol{R'}$, so that we expect only elastic scattering from the Mott insulator.

We can estimate the scale of the Mott insulator's inelastic background more precisely by using the harmonic approximation of the Wannier function, in which we substitute the ground state of the harmonic approximation to the bottom of an individual well in the lattice. Near to the central peak, the inelastic background decays exponentially with the lattice strength, as $\exp\left(-\frac{\pi^2}{2}\sqrt{\frac{V_o}{E_r}}(j-l)^2\right)$, where j and l ($j \neq l$) are positions of lattice sites in units of lattice spacings. For lattice depths in the typical range $V_o \leq 30E_r$, the inelastic contribution is strongly suppressed even for incident probe energies that exceed the gap energy. This contrasts markedly with the superfluid cross section, which carries a prominent inelastic background that scales as the number of atoms in the lattice. In the regions between the Bragg peaks, this background serves as an unambiguous indicator of the many body phase of the lattice.

We have also examined the disappearance of the superfluid inelastic background as the interaction strength between the lattice atoms is increased. This required that we calculate scattering cross sections for arbitrary values of the parameter U/J. At intermediate values, this requires knowledge of the spectrum of the Bose Hubbard Hamiltonian. We calculated the matrix elements of the density operator by exactly diagonalizing the Bose Hubbard Hamiltonian for small lattices. Using these results, we have shown the angular cross section given in (2) for several values of U/J in Fig. 2. At $U/J = 0$ the numerical result coincides with the analytic result we presented. The inelastic background that scales as the number of atoms is present. This inelastic background decays to zero as the interaction strength is increased, and the cross section converges on the analytic result we gave for the Mott insulator. We note that the amplitude of the inelastic background has decayed by more than half at $U/J = 4$. For $U/J = 8$, the background is largely gone. This coincides with the range over which the superfluid fraction vanishes [5].

Our analytic results for the scattering cross section when the interaction strength dominates the tunneling matrix element ($U \gg J$) and vice versa show that the many body phase in the lattice strongly affects the scattering cross section of a low-energy matter wave probe. The periodic nature of the target gives rise in both many body phases to coherent Bragg peaks whose height scales as the square of the number of atoms in the lattice. In addition, an inelastic background determined by the excitation spectrum of the target serves as an indicator of the presence of superfluidity, and scales as the number of atoms in the target. This provides an easily identifiable signature of the many body phase.

Matter waves offer an effective method for non-destructively probing the many body phase in an optical lattice. More broadly, the scattering of matter waves depends strongly on properties such as the distribution of atoms in a partially filled lattice, and on the long range correlations and other manifestly quantum mechanical effects found in this novel state of matter. This makes this technique well-suited for examining a range of phenomena, including the effect of inhomogeneity of bosons and fermions and disorder in the lattice, in addition to probing the many body quantum phase transition.

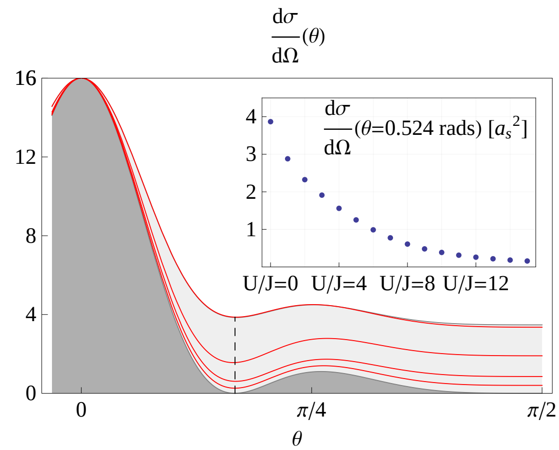

FIG. 2: Cross sections for a probe with initial energy $(\hbar k_o)^2/(2m) = E_r$, a lattice of depth $V_o = 15E_r$, with 4 atoms and 4 sites, and $J = 0.002$. The values of U/J shown are: 0, 4, 8, and 16. The superfluid analytic result (light gray) for the inelastic background scales as N. The corresponding background for the Mott insulator (dark gray) is strongly suppressed. The inset shows the numerical cross section at the vertical dashed line as a function of U/J.

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